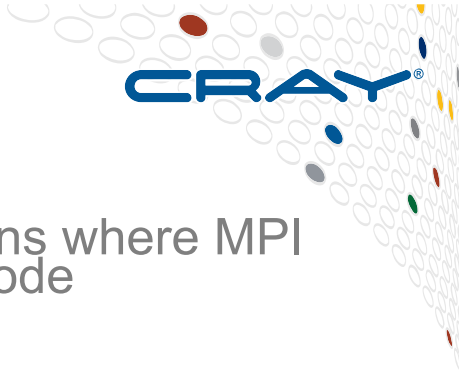
Threading on the Node

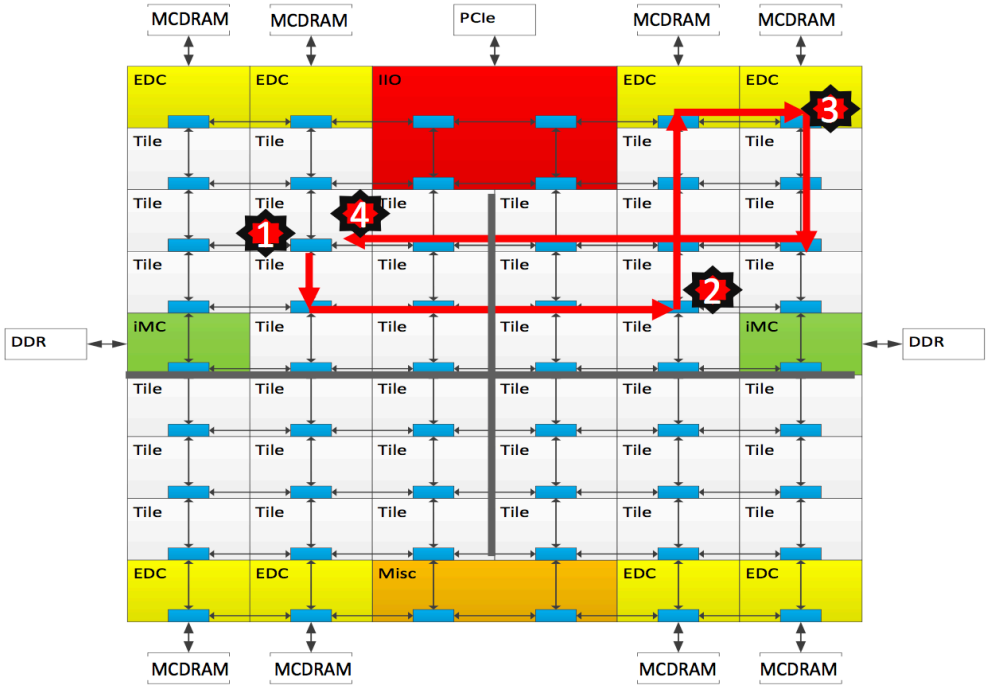
OpenMP works great if it is implemented correctly

Looking at KNL



- **Lots of cores**
  - While MPI can run across all the cores, there are situations where MPI hits bottlenecks due to the number of MPI tasks on the node
  - We ALWAYS want to run multiple MPI tasks on the node
  - Want to identify a MPI sweet spot
  - A good guide is to start with a MPI task on each NUMA region
- **OpenMP**
  - Traditional approach has many short-comings
    - Requires a lot of code modifications
      - Lots of Comment Line directives
      - Does not deal with locality
      - Difficult to load balance
  - Is there a better way?
    - SPMD OpenMP
      - Fewer code modifications
      - Requires a better understanding of threads
- **KNL has NUMA issues**

Cluster Mode: Quadrant



Chip divided into four virtual Quadrants

Address hashed to a Directory in the same quadrant as the Memory

Affinity between the Directory and Memory

Lower latency and higher BW than all-to-all. SW Transparent.

1) L2 miss, 2) Directory access, 3) Memory access, 4) Data return

Why does all-MPI work well on multi/many core architectures?

- **All MPI forces locality**
  - Each MPI task allocated/utilizes memory within the NUMA region that it is running in.
- **All MPI allows tasks to run asynchronously**
  - This allows very good sharing of the memory bandwidth available on the node
  - We have found that KNL Quadrant mode is very good for all-MPI due to the memory bandwidth sharing to all memories
- **One MPI disadvantage is that re-distributing work is difficult and inefficient**
  - Have to move a lot of data

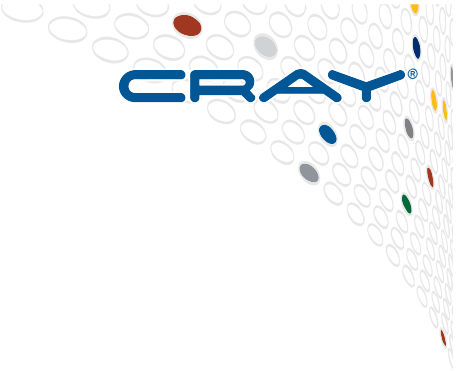
Can we take clues from all-MPI advantages and disadvantages to design a good OpenMP code?

- **Can we force locality like MPI does?**
  - MPI forces each MPI task to allocate the data that it uses.
  - Tradition OpenMP has no notion of locality
- **Can we allow threads to work asynchronously?**
  - MPI only barriers when messages are exchanged
  - Tradition OpenMP implies barriers after a parallel region
  - Loop level parallelism forces too much synchronization
- **Can we somehow control scheduling of the threads to enable more dynamic re-distribution of work**

Can we force locality like MPI does?

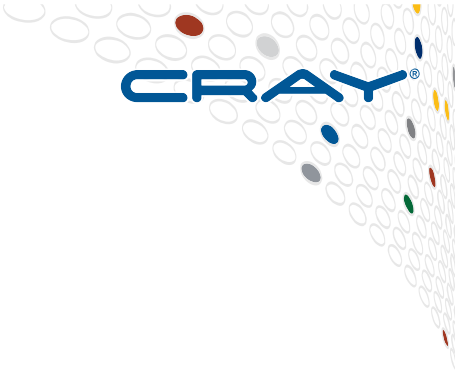
- **Introduce a high level !$OMP PARALLEL region**
  - Down the call chain the user is responsible for managing threads
    - Initialize shared data within the !$OMP PARALLEL region, each thread allocates the data it will be using
    - Application developer must assure that shared data is shared as in the Fortran/C/C++ convention
      - This can be an issue down the call chain, when a shared local variable is required; that is, a reduction variable
    - Application developer must assure that private data is allocated on stack as with the Fortran and C conventions

What if you need a shared variable down the call chain



```
Subroutine within_a_parallel( )

Real, pointer ::  shared_p( : )

!$omp single
allocate(shared_p(0:100))
!$omp end single copyprivate(share_p)

…

End subroutine
```

Can we allow threads to work asynchronously?



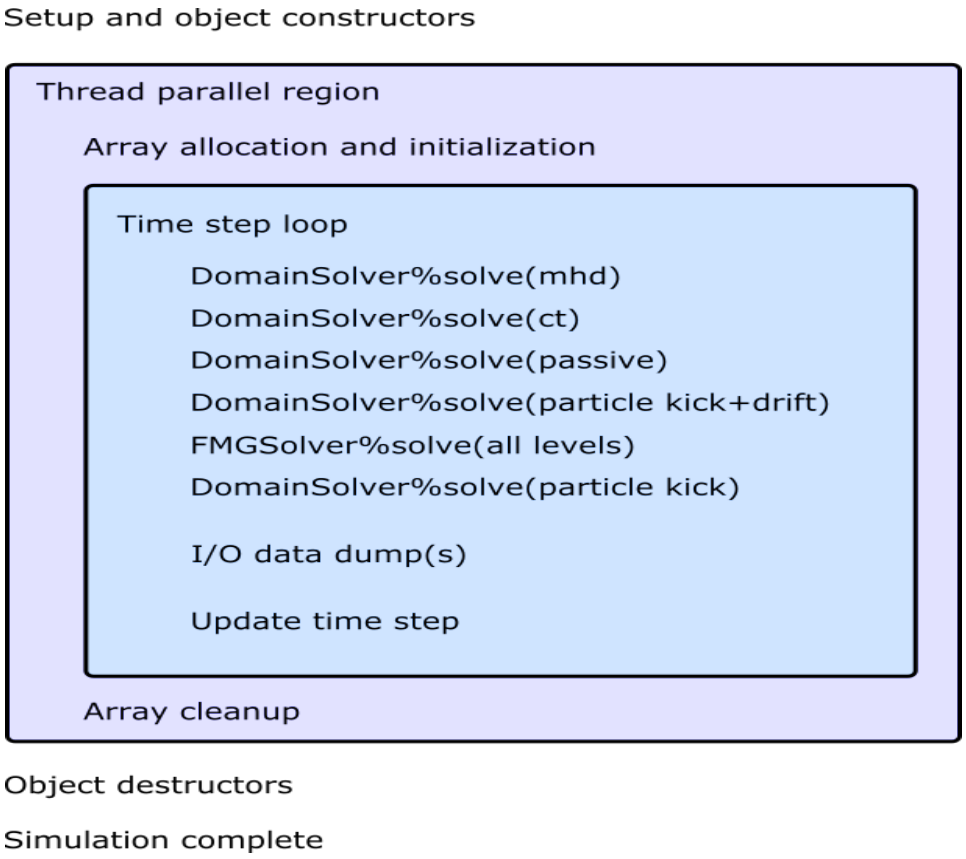
- **Must minimize sychronization**
  - Calling un-treaded routines
    - Must extend concept to all computational kernels
    - You can have replicated computation across the threads
  - Calling library routines
    - Can each thread call a un-threaded library routine
    - If library routine is threaded – must barrier prior to and after call
  - Calling MPI
    - Consider having each thread do it own message passing
      - Example coming

High-level OpenMP and Thread Scalable MPI-RMA:

Application Study with the Wombat Astrophysical MHD Code

Dr. Peter Mendygral
Cray Inc.

Wombat Driver and Parallel Region

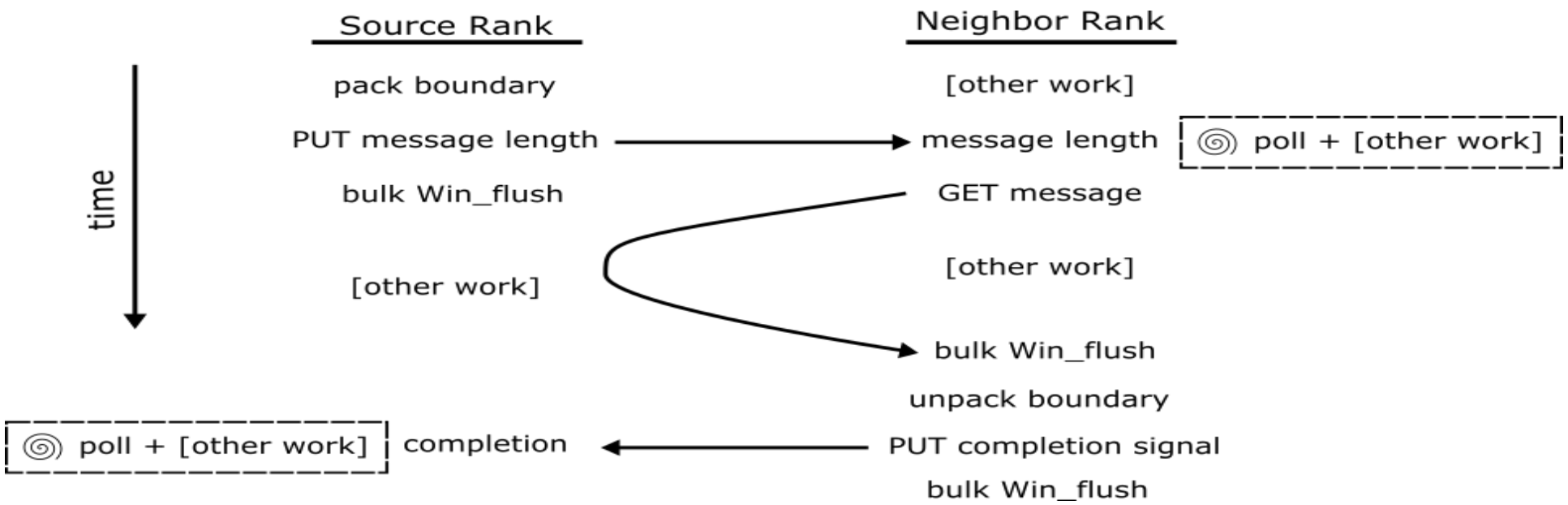


Communication Concerns

- **If a rank is made much wider with threads, serialization around MPI will limit thread scaling and overall performance**
  - Nearly all MPI libraries implement thread safety with a global lock
  - Cray is addressing this issue
    - Released per-object lock library
    - Threading enhancements under design now for two-sided (released per-object lock library a first step)
- **Wide OpenMP also means more communication to process**
  - Every Patch now has its own smaller boundaries to communicate
  - Starts tipping the behavior towards the message rate limit
  - Two-sided tag matching cannot be done in parallel and will limit thread scaling
    - May start hitting tag limit
- **Slower serial performance of KNL => maybe look for the lightest weight MPI layer available**
  - MPI-RMA over DMAPP on Cray systems is a thin software layer that achieves similar performance to SHMEM

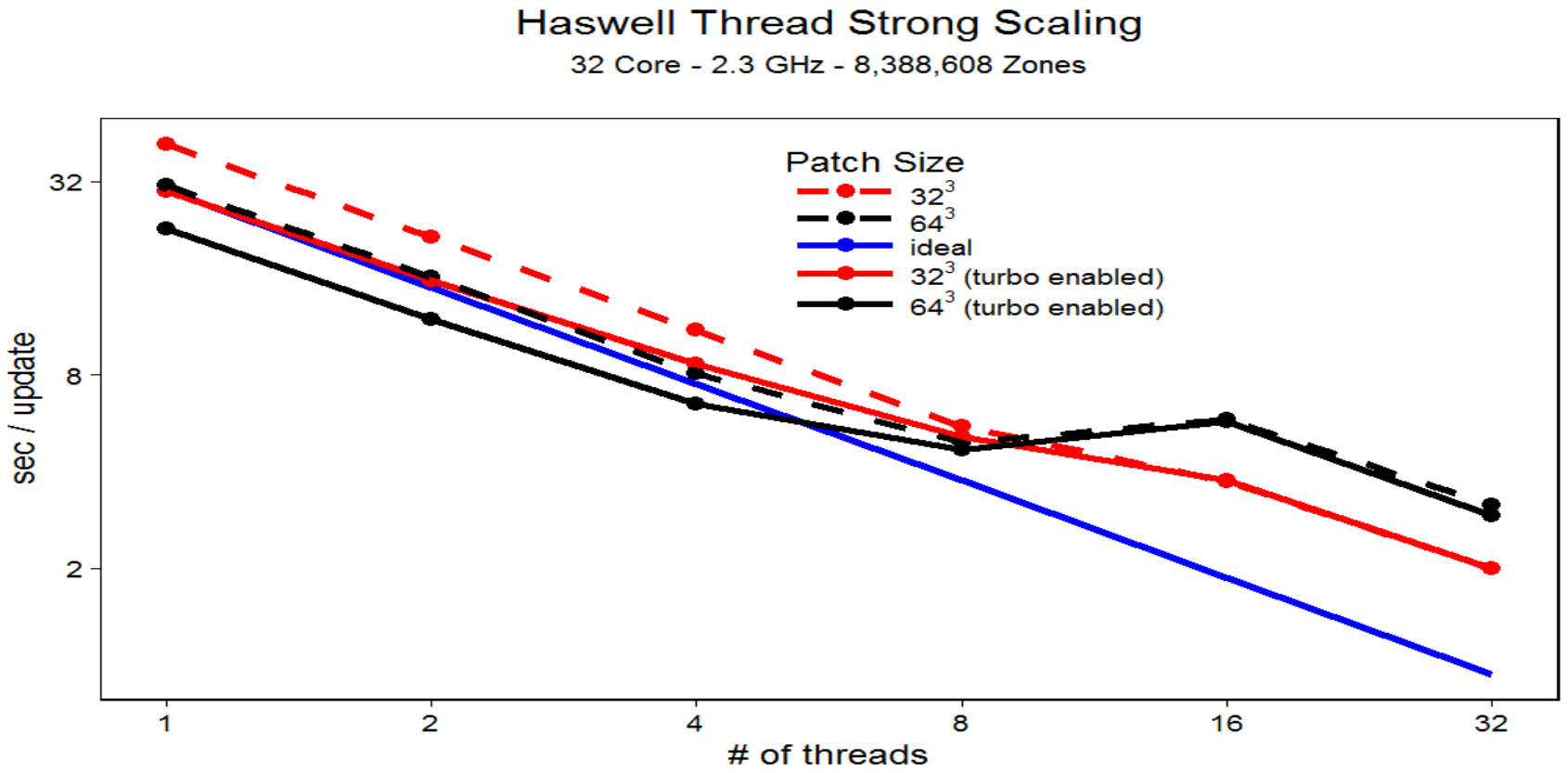
RMA Boundary Communication Cycle

- **Single passive RMA exposure epoch used for the duration of the application**
  - No explicit synchronization between ranks
  - RMA semantics make computation/communication overlap simpler to achieve

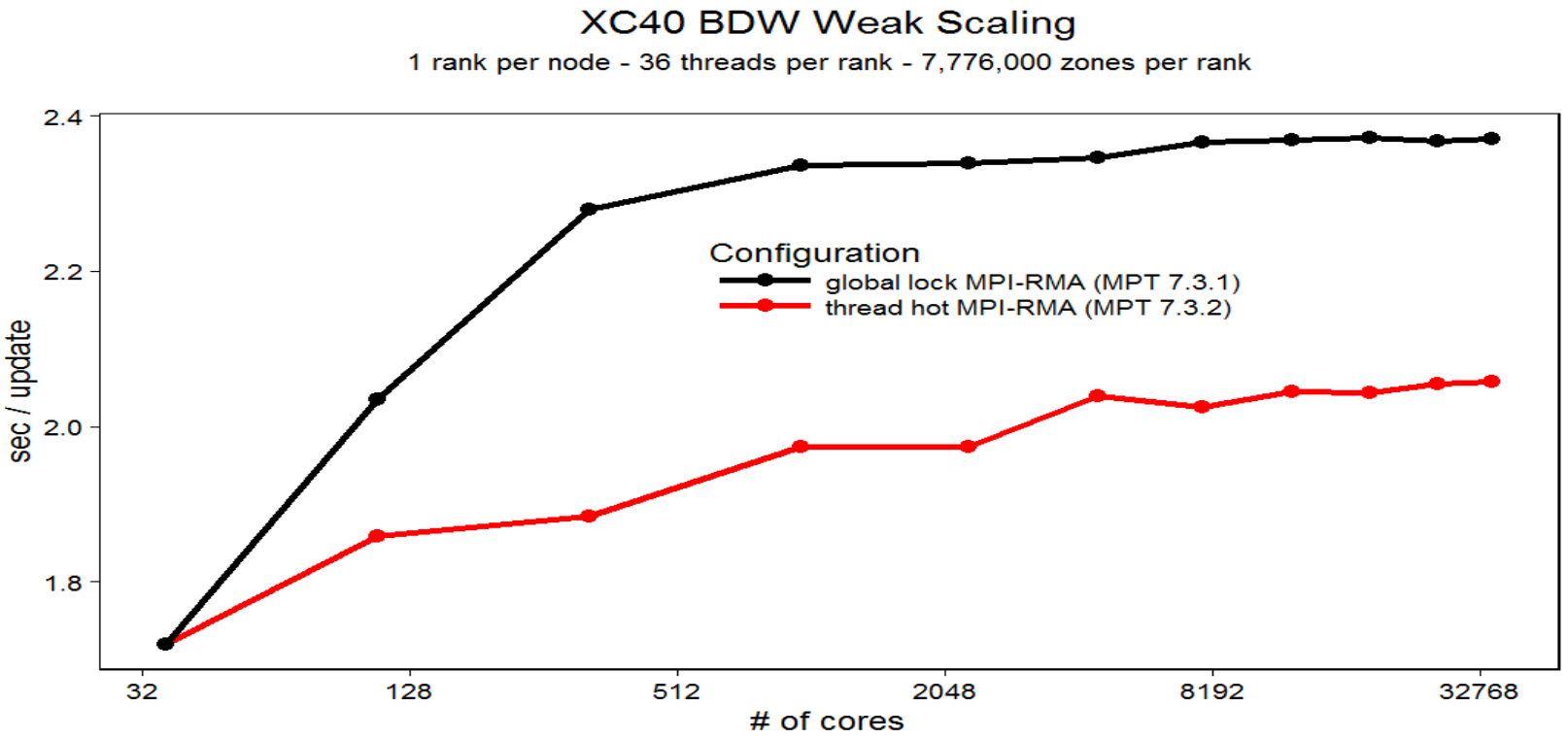


Thread Hot MPI-RMA

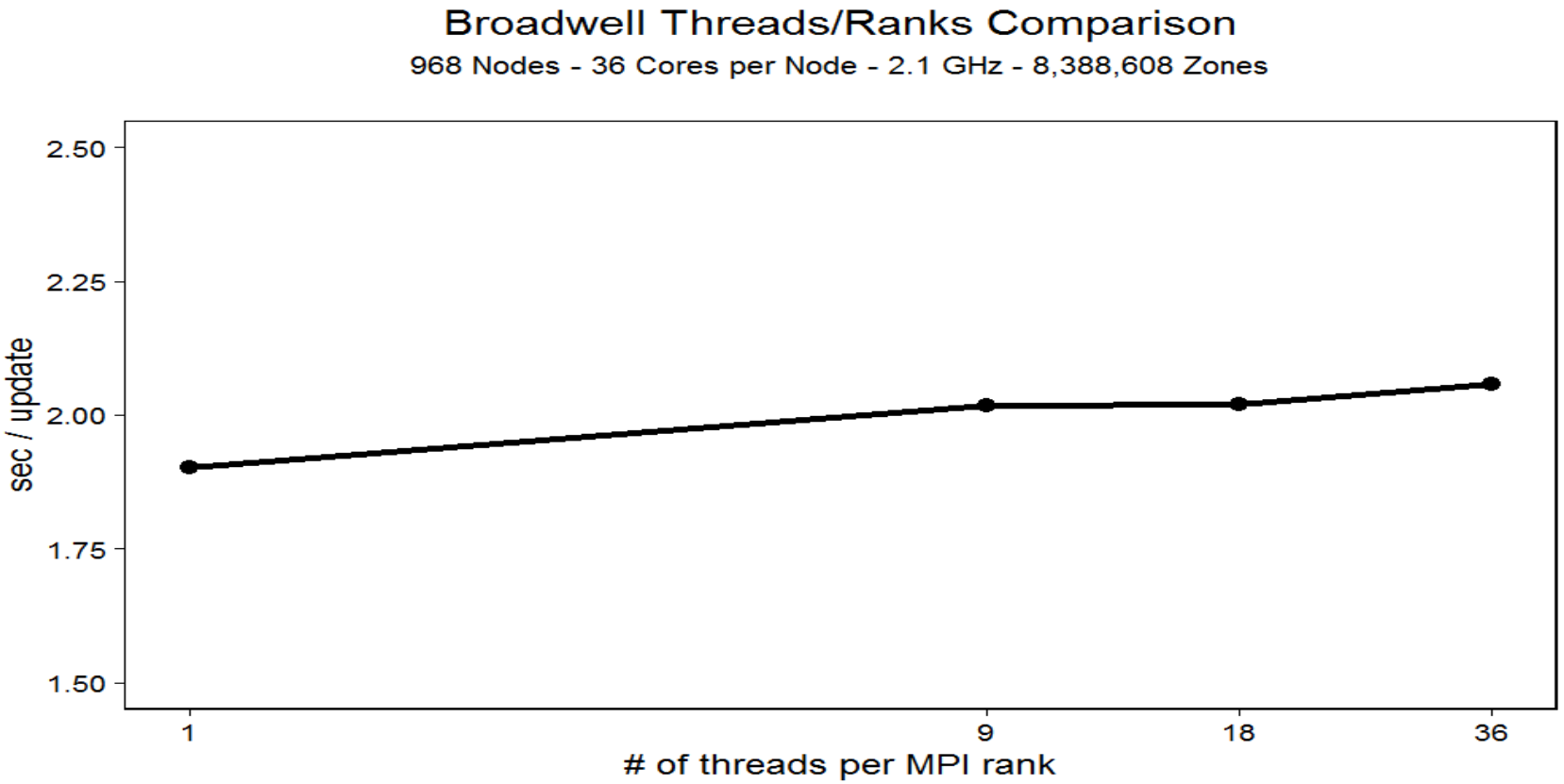
- **DMAPP library was enhanced to be "thread hot" for SHMEM**
  - "thread hot" is more than "thread safe"
  - "thread hot" implies concurrency and performance across threads was central to the design
- **MPI-RMA over DMAPP leverages this feature as of MPT 7.3.2**
  - No locks used in DMAPP layer
  - Very light weight locking in MPI layer
  - Design makes it very likely that locks are uncontended
  - Network resources efficiently managed among threads
  - Performance approaches that of N independent processes when using N threads
- **Example on HSW with 16 threads each on 2 nodes**
  - OSU passive MPI_Put bandwidth for 8 B message
  - MPT 7.3.1 = 5.27 MB/s
  - MPT 7.3.2 = 399.9 MB/s
  - 75X improvement



- **Tunable Patch size very important to performance**



- **Rank reordering**
  - Cartesian domain optimization for XC topology/placement improves largest run wall time by additional 2.3%



- Less than 8% difference between 1 and 36 threads per rank
- Ideal for application like Wombat is 0%

Can we somehow control scheduling of the threads to enable more dynamic re-distribution of work

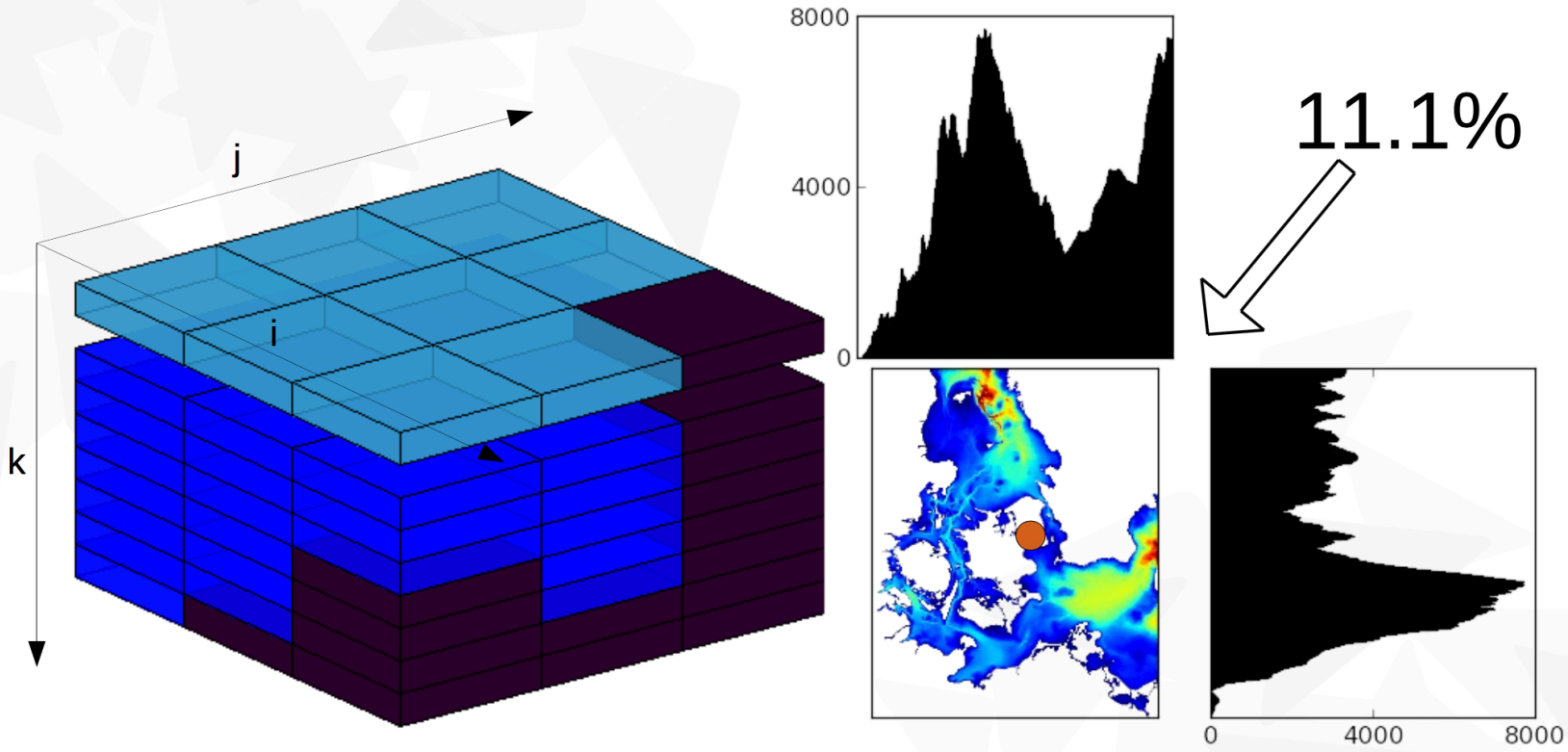
- **With SPMD OpenMP, the user can take the responsibility for allocating the work to the threads**
  - Can be simple chunking
  - Can understand the scarcity of the problem and allocate work accordingly
  - Can dynamically use runtime statistics to address load-imbalance

HBM code modernization -

insights from a Xeon Phi experiment

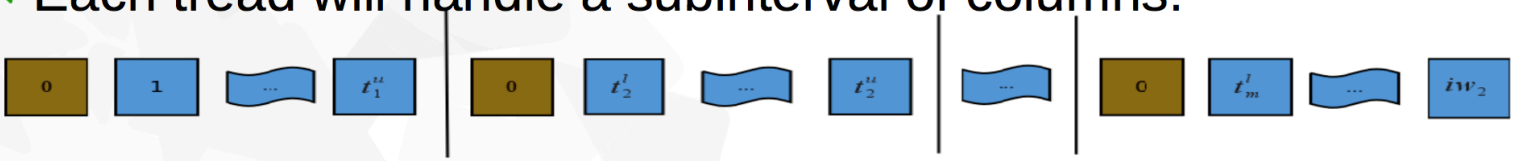
Jacob Weismann Poulsen, DMI, Denmark
Per Berg, DMI, Denmark
Karthik Raman, Intel, USA

The data is sparse and highly irregular



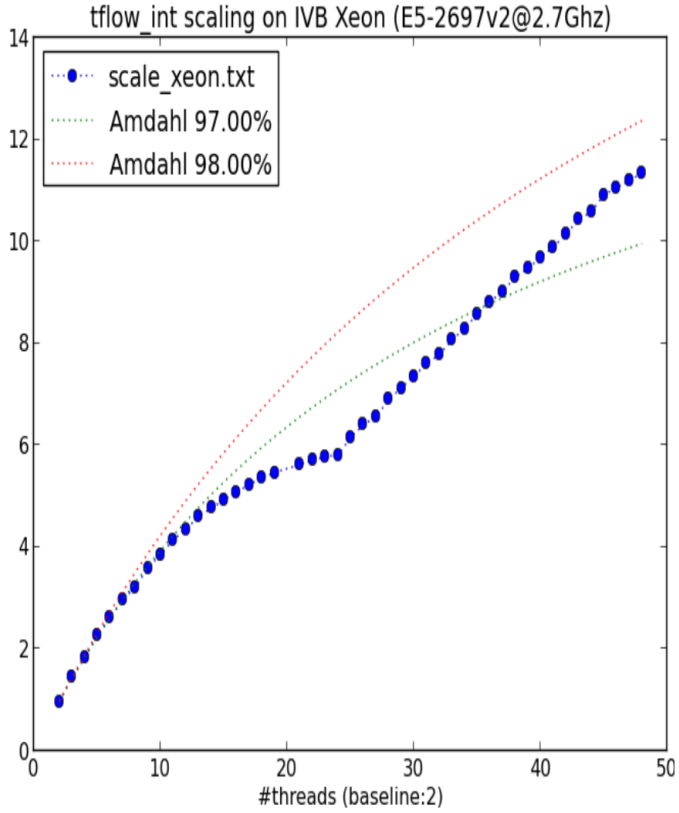
Data layout for threads (or tasks + explicit halo)

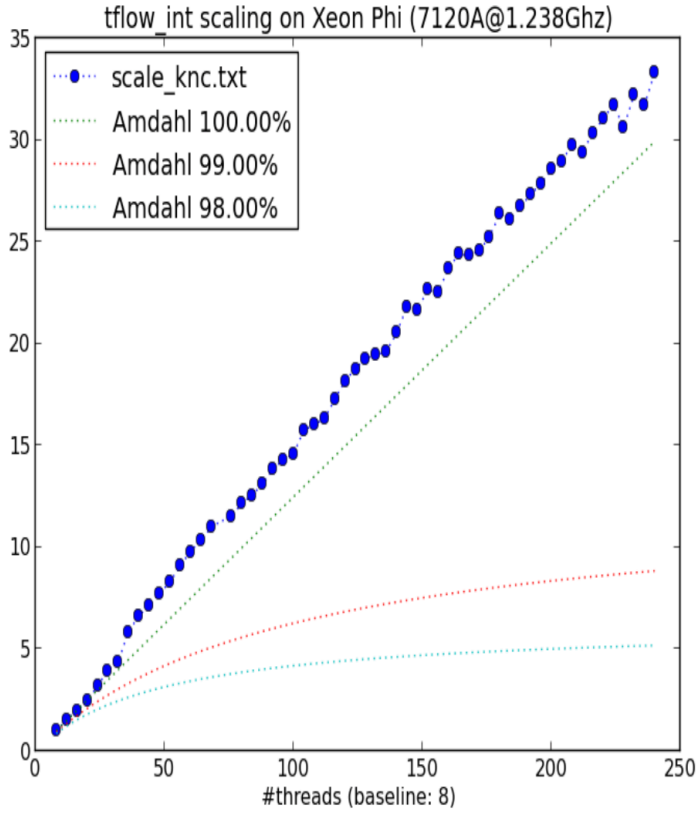
- Each tread will handle a subinterval of columns:



- Another layout of the columns will impose another decomposition for the threads (and the tasks).

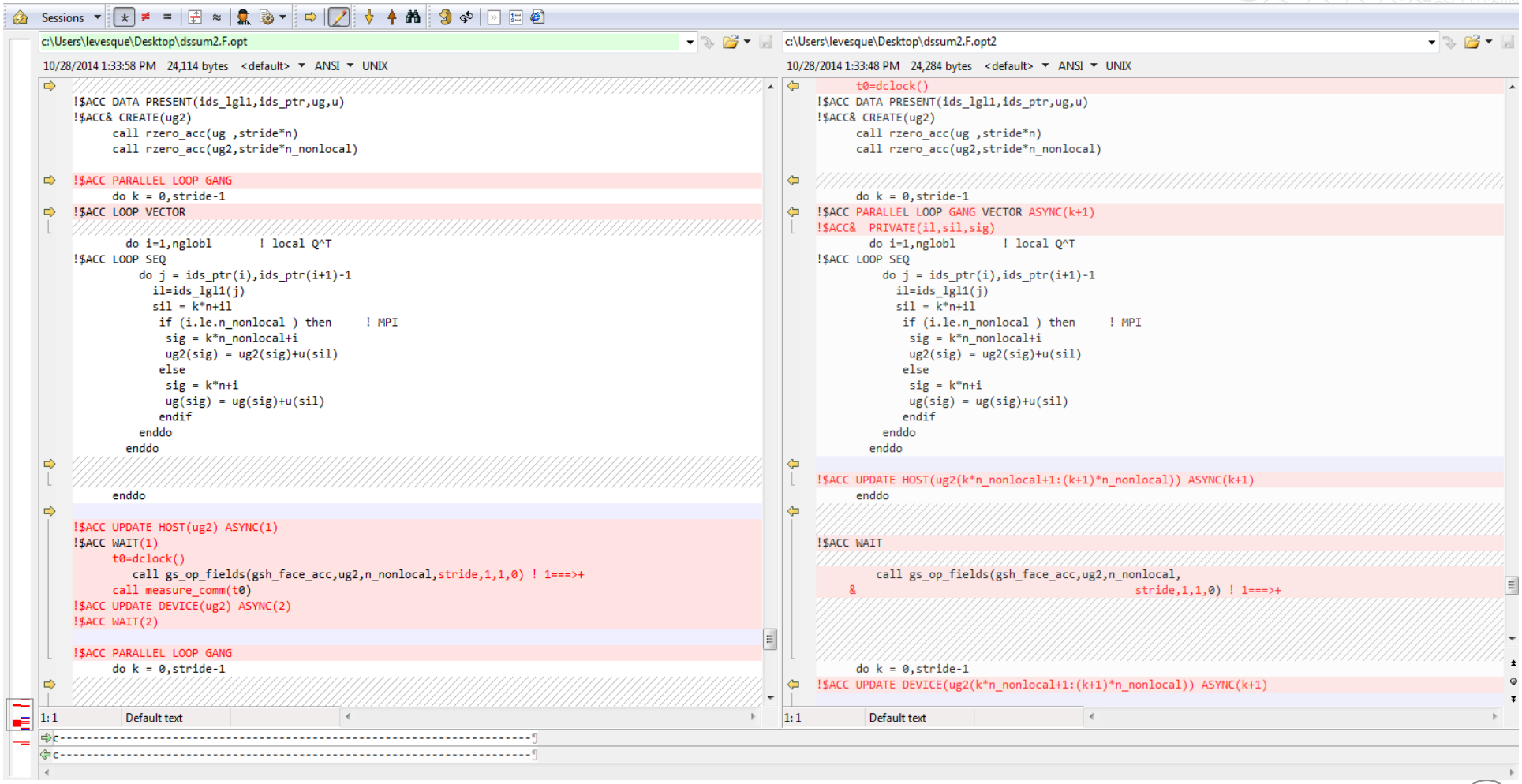
```
...
!$OMP PARALLEL DEFAULT(SHARED)
call foo( ... );call bar(...); ...
!$OMP BARRIER
call halo_update(...)
!$OMP BARRIER
call baz( ... );call quux(...); ...
!$OMP END PARALLEL
...
subroutine foo(...)
  ...
  call domp_get_domain(kh, 1, iw2, nl, nu, idx)
  do iw=nl,nu
    i = ind(1,iw)
    j = ind(2,iw)
    ! all threadlocal wet-points (:,:,:) are reached here
    ...
  enddo
```


tflow_int scaling on IVB Xeon (E5-2697v2@2.7Ghz)
scale_xeon.txt
Amdahl 97.00%
Amdahl 98.00%
#threads (baseline:2)


tflow_int scaling on Xeon Phi (7120A@1.238Ghz)
scale_knc.txt
Amdahl 100.00%
Amdahl 99.00%
Amdahl 98.00%
#threads (baseline: 8)

What about performance portability

- **When running S3D on Titan we used Cuda Streams extensively**
  - Consider using the 16 Cuda streams for the 16 threads within the SPMD unit.


Sessions
c:\Users\levesque\Desktop\dssum2.F.opt
10/28/2014 1:33:58 PM 24,114 bytes <default> ANSI UNIX
!$ACC DATA PRESENT(ids_lgl1,ids_ptr,ug,u)
!$ACC& CREATE(ug2)
call rzero_acc(ug ,stride*n)
call rzero_acc(ug2,stride*n_nonlocal)
!$ACC PARALLEL LOOP GANG
do k = 0,stride-1
!$ACC LOOP VECTOR
do i=1,nglobl ! local Q^T
!$ACC LOOP SEQ
do j = ids_ptr(i),ids_ptr(i+1)-1
il=ids_lgl1(j)
sil = k*n+il
if (i.le.n_nonlocal) then ! MPI
sig = k*n_nonlocal+i
ug2(sig) = ug2(sig)+u(sil)
else
sig = k*n+i
ug(sig) = ug(sig)+u(sil)
endif
enddo
enddo
enddo
!$ACC UPDATE HOST(ug2) ASYNC(1)
!$ACC WAIT(1)
t0=dclock()
call gs_op_fields(gsh_face_acc,ug2,n_nonlocal,stride,1,1,0) ! 1===>+
call measure_comm(t0)
!$ACC UPDATE DEVICE(ug2) ASYNC(2)
!$ACC WAIT(2)
!$ACC PARALLEL LOOP GANG
do k = 0,stride-1
1: 1
Default text
c:\Users\levesque\Desktop\dssum2.F.opt2
10/28/2014 1:33:48 PM 24,284 bytes <default> ANSI UNIX
t0=dclock()
!$ACC DATA PRESENT(ids_lgl1,ids_ptr,ug,u)
!$ACC& CREATE(ug2)
call rzero_acc(ug ,stride*n)
call rzero_acc(ug2,stride*n_nonlocal)
do k = 0,stride-1
!$ACC PARALLEL LOOP GANG VECTOR ASYNC(k+1)
!$ACC& PRIVATE(il,sil,sig)
do i=1,nglobl ! local Q^T
!$ACC LOOP SEQ
do j = ids_ptr(i),ids_ptr(i+1)-1
il=ids_lgl1(j)
sil = k*n+il
if (i.le.n_nonlocal) then ! MPI
sig = k*n_nonlocal+i
ug2(sig) = ug2(sig)+u(sil)
else
sig = k*n+i
ug(sig) = ug(sig)+u(sil)
endif
enddo
enddo
!$ACC UPDATE HOST(ug2(k*n_nonlocal+1:(k+1)*n_nonlocal)) ASYNC(k+1)
enddo
!$ACC WAIT
call gs_op_fields(gsh_face_acc,ug2,n_nonlocal,
& stride,1,1,0) ! 1===>+
do k = 0,stride-1
!$ACC UPDATE DEVICE(ug2(k*n_nonlocal+1:(k+1)*n_nonlocal)) ASYNC(k+1)
1: 1
Default text

Example of Cuda Streams (1)

```
!$ACC DATA PRESENT(ids_lgl1,ids_ptr,ug,u)
!$ACC& CREATE(ug2)
      call rzero_acc(ug ,stride*n)
      call rzero_acc(ug2,stride*n_nonlocal)

      do k = 0,stride-1
!$ACC PARALLEL LOOP GANG VECTOR ASYNC(k+1)
!$ACC&  PRIVATE(il,sil,sig)
        do i=1,nglobl       ! local Q^T
!$ACC LOOP SEQ
          do j = ids_ptr(i),ids_ptr(i+1)-1
            il=ids_lgl1(j)
            sil = k*n+il
             if (i.le.n_nonlocal ) then     ! MPI
              sig = k*n_nonlocal+i
              ug2(sig) = ug2(sig)+u(sil)
             else
              sig = k*n+i
              ug(sig) = ug(sig)+u(sil)
             endif
          enddo
        enddo
!$ACC UPDATE HOST(ug2(k*n_nonlocal+1:(k+1)*n_nonlocal)) ASYNC(k+1)
      enddo
!$ACC WAIT
```

Example of Cuda Streams (2)

```
do k = 0,stride-1
!$ACC UPDATE DEVICE(ug2(k*n_nonlocal+1:(k+1)*n_nonlocal)) ASYNC(k+1)

!$ACC PARALLEL LOOP GANG VECTOR ASYNC(k+1)
!$ACC&  PRIVATE(il,sil,sig)
       do i=1,nglobl       ! local Q
!$ACC LOOP SEQ
         do j = ids_ptr(i),ids_ptr(i+1)-1
           il = ids_lgl1(j)
           sil = k*n+il
           if (i.le.n_nonlocal ) then     ! MPI
            sig = k*n_nonlocal+i
            u(sil) = ug2(sig)
           else
           sig = k*n+i
           u(sil) = ug(sig)
           endif
         enddo
       enddo
     enddo
!$ACC WAIT
!$ACC END DATA
```

Conclusion

- **To scale well on many/multi-core systems, application developers must develop efficient threading**
  - Must pay attention to NUMA regions
  - Must avoid overhead caused by
    - Too much synchronization
    - Load imbalance
- **On some systems all-MPI will perform very well and will out-perform poorly implemented OpenMP**
  - Not performance portable to hosted accelerators
- **SPMD or Wide OpenMP is an alternative**
  - Application developers have all the power to generate difficult to find race conditions, must understand the implications of high level threading